

LIANG WANG

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Education

National University of Singapore

Visiting Ph.D. Student

Singapore

2025 - 2026 (expected)

- Lab: [ZhangLab/DeepMed](#), focusing on AI for Science
- Advisor: Prof. [Yang Zhang](#) Mentor: Dr. [Zhiyuan Liu](#)
- Research Interests: Multi-modal Molecular Generation, Diffusion Models, Multi-modal LLMs

Institution of Automation, Chinese Academy of Sciences

Ph.D. in Pattern Recognition and Intelligent Systems (selected for the PhD honors program)

Beijing, China

2021 - 2026 (expected)

- Lab: Center for Research on Intelligent Perception and Computing ([CRIPAC](#)), State Key Laboratory of Multimodal Artificial Intelligence Systems ([MAIS](#))
- Advisor: Prof. [Liang Wang](#) Co-advisors: Prof. [Shu Wu](#) and Prof. [Qiang Liu](#)
- Research Interests: AI for Science, Graph Machine Learning, Data Mining

Tongji University

B.Eng. in Software Engineering

Shanghai, China

2017 - 2021

- GPA: 4.86/5.00 (Ranking 3/214, Top 1.4%)
- Honors and Awards: National Scholarship (Top 1%), Outstanding Graduate of Shanghai (Top 5%)

Selected Publications

MolSpectra: Pre-training 3D Molecular Representation with Multi-modal Energy Spectra

- [Liang Wang](#), Shaozhen Liu, Yu Rong, Deli Zhao, Qiang Liu, Shu Wu, Liang Wang
- *ICLR 2025*

Pin-Tuning: Parameter-Efficient In-Context Tuning for Few-Shot Molecular Property Prediction

- [Liang Wang](#), Qiang Liu, Shaozhen Liu, Xin Sun, Shu Wu, Liang Wang
- *NeurIPS 2024*

Rethinking Graph Masked Autoencoders through Alignment and Uniformity

- [Liang Wang](#)^{*}, Xiang Tao^{*}, Qiang Liu, Shu Wu, Liang Wang
- *AAAI 2024*

DIVE: Subgraph Disagreement for Graph Out-of-Distribution Generalization

- Xin Sun, [Liang Wang](#), Qiang Liu, Shu Wu, Zilei Wang, Liang Wang
- *KDD 2024*

GSLB: The Graph Structure Learning Benchmark

- Zhixun Li, [Liang Wang](#), Xin Sun, Yifan Luo, Yanqiao Zhu, Dingshuo Chen, Yingtao Luo, Xiangxin Zhou, Qiang Liu, Shu Wu, Liang Wang, Jeffrey Xu Yu
- *NeurIPS 2023*

Bi-Level Graph Structure Learning for Next POI Recommendation

- [Liang Wang](#), Shu Wu, Qiang Liu, Yanqiao Zhu, Xiang Tao, Mengdi Zhang, Liang Wang
- *IEEE Transactions on Knowledge and Data Engineering 2024*

Semantic Evolvment Enhanced Graph Autoencoder for Rumor Detection

- Xiang Tao, [Liang Wang](#), Qiang Liu, Shu Wu, Liang Wang
- *WWW 2024*

Chain-of-History Reasoning for Temporal Knowledge Graph Forecasting

- Yuwei Xia, Ding Wang, Qiang Liu, [Liang Wang](#), Shu Wu, Xiaoyu Zhang
- *ACL 2024 (Findings)*

Selected Projects

PyGCL: A PyTorch Library for Graph Contrastive Learning

<https://github.com/PyGCL/PyGCL>

- ☆ Github Star: 919
- An easy-to-use library for graph contrastive learning with PyTorch. It implements a wide variety of contrastive objectives, data augmentations, contrasting modes and other utilities useful for implementing and evaluating contrastive learning on graphs.

GSLB: A Benchmark of Graph Structure Learning

<https://github.com/GSL-Benchmark/GSLB>

- ☆ Github Star: 112
- An open-source library built for easy implementation and evaluation of graph structure learning model family. It offers a versatile control of graph dataset loading, structure learners, structure processors, and a bunch of reproduced models.

Internship

AI4Science Group, Alibaba DAMO Academy

Hangzhou, China

Research Intern

Aug. 2024 - Mar. 2025

- Advised by Dr. [Yu Rong](#) and Dr. [Tingyang Xu](#).
- Conducted research on AI for chemistry and life science. The research work has been published in ICLR 2025.

Graph Learning Group, NLP Center, Meituan Inc.

Beijing, China

Research Intern

Sept. 2021 - Oct. 2022

- Conducted research on graph self-supervised learning and graph-based spatial-temporal data mining. The research works have been published in IEEE TKDE and SDM 2024.

Advertising Department, ByteDance Inc.

Shanghai, China

Machine Learning Engineer Intern

Jul. 2020 - Dec. 2020

- Supported the improvement of advertising machine learning models, and the development of the advertising system.

Talks

Molecular Spectroscopy, at Alibaba DAMO Academy, 2024, [Slides](#)

Molecular Representation Learning and Property Prediction, Invited by DP Technology, 2024, [Slides](#)

Denoising-based 3D Molecular Pre-training, 2024, [Slides](#)

Generative Graph Self-Supervised Learning, 2023, [Slides](#)

Graph Transformers, 2022, [Slides](#)

Graph Self-Supervised Learning and Pre-Training, 2021, [Slides](#)

Academic Services

Conference Reviewers: NeurIPS 2024 2025, ICLR 2025, ICML 2025, KDD 2024 2025, AISTATS 2025

Journal Reviewers: IEEE TKDE

Technical Skills

Programming Languages: Python, C++, Matlab, Java, C#

Machine Learning Frameworks: PyTorch, PyTorch Geometric (PyG), Deep Graph Library (DGL)

Others: L^AT_EX, Git